QUANTIZATION OF SINGULAR SYSTEMS AND INCOMPLETE MOTIONS

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The need for a mathematically rigorous quantization procedure of singular spaces and incomplete motions is pointed out in connection with quantum cosmology. We put our previous suggestion for such a procedure, based on the theory of induced representations of C^*-algebras, in the light of L. Schwartz' theory of Hilbert subspaces. This turns out to account for the freedom in the induction procedure, at the same time providing a basis for generalized eigenfunction expansions pertinent to the needs of quantum cosmology. Reinforcing our previous proposal for the wave-function of the Universe, we are now able to add a concrete prescription for its calculation.

1 Introduction

1.1 Incomplete dynamical systems

Minisuperspace cosmologies with singularities are examples of dynamical systems whose motion may be incomplete (that is, *in a given parametrization* the flow may not be defined for all $t \in \mathbb{R}$). In general, classical incomplete motion may occur even on smooth phase spaces; for example, a particle may escape to infinity in a finite time. In cosmological examples, though, the incompleteness is generically caused by the presence of singularities in the space of physical degrees of freedom of the model in question. The notion of singularity used here is rather wide; boundary points to a manifold are included as possible singular points. Indeed, the incompleteness of the motion of a cricket ball off a batsman hitting a boundary is precisely caused by the boundary of the field. On the other hand, one may think of the incompleteness of the motion of an observer falling into a black hole. The question whether the space is question may be extended so as to render the given motion complete is interesting, but not quite relevant in this context.

In the general theory of dynamical systems, incompleteness is not much studied, for the simple reason that under mild conditions one may reparametrize the flow, so as to make the motion complete. The question whether a singularity is approached in finite time therefore appears to be ill-defined. However, the physics of the situation usually singles out a preferred choice of the time co-ordinate, an issue that has been much discussed in classical and quantum

gravity; see Isham [1] and references therein.

In our opinion, in a canonical context the choice of a time parameter is determined by the choice of the physical Hamiltonian, which simply defines time through Hamilton's equations. Hence the above question in any case makes sense in the setting of *Hamiltonian* dynamical systems. Further to the well-studied classes of integrable and chaotic systems, one should therefore study the class of incomplete Hamiltonian dynamical systems. While this is fascinating already classically, the issue of genuine physical importance lies in the quantum theory of such systems. It is well known that, in view of the unitarity of the time-evolution, a quantum system can be neither chaotic (in the classical sense) nor incomplete. Hence one faces the difficult task of identifying properties of the quantum Hamiltonian which indicate that the classical limit of the theory is integrable, chaotic, or incomplete. Signatures for chaos are found in the statistical distribution of the eigenvalues, whereas classical incompleteness is often related to the fact that the Hamiltonian fails to be essentially self-adjoint on its natural domain of smooth compactly supported wave-functions [2]. It is intuitively evident why this is so: such wave-functions have support away from the singularities, so that the natural domain contains no information about the boundary conditions [3].

1.2 Singular reduction

Our second source of inspiration lies in the origin of the singularities of the physical phase space of general relativity. Namely, since the space of unphysical degrees of freedom (in whatever formalism one uses) is regular, the singularities come from the constraints of Einstein gravity. The singularities of the reduced phase space are well understood: the physical phase space is stratified by symplectic manifolds, each of which is stable under the Hamiltonian flow generated by any function that Poisson-commutes with all constraints [4]. This important infinite-dimensional fact is entirely analogous to the case of singular Marsden-Weinstein quotients by proper actions of finite-dimensional Lie groups on finite-dimensional symplectic manifolds [5].

When the symplectic space one starts from is a cotangent bundle $S = T^*Q$, and the group action on S (with equivariant momentum map J) is pulled back from a G-action on Q, the Marsden-Weinstein quotient at zero is simply $J^{-1}(0)/G = T^*(Q/G)$, where away from the singular points the cotangent bundle is defined as usual, whereas at the singular points it is defined by the left-hand side. One may quantize the reduced space by saying that the pertinent Hilbert space is $L^2(Q/G)$, and that the Hamiltonian is minus the Laplacian, defined on the domain $C_c^\infty(Q/G)$ [6]. As already mentioned in the

previous subsection, this operator is not essentially self-adjoint; one needs to choose boundary conditions, so there is no unique quantum theory.

Instead, one needs a method of constrained quantization which parallels the classical procedure of symplectic reduction, and which still applies when the usual conditions guaranteeing that the reduced space be smooth [5] do not apply. The method proposed by the author [7,8,9] satisfies these requirements, and simultaneously solves the problem described in the previous paragraph.

The essence of this method is best explained by comparing it with Dirac's well-known technique of constrained quantization [10]. We restrict ourselves to first-class constraints. Recall that symplectic reduction is a two-step procedure: firstly, the constraints $\varphi_i = 0$ are imposed, and secondly, roughly speaking, gauge-equivalent points on the constraint hypersurface are identified. In quantum theory only one of these steps has to be taken. Dirac's approach to constrained quantization selects the first step, in imposing the quantized constraints $\hat{\varphi}_i$ as state conditions $\hat{\varphi}_i \Psi = 0$ on the Hilbert space $\mathcal{H}$ of the unconstrained system.

These equations rarely have solutions in $\mathcal{H}$, and are, accordingly, usually solved in some enlargement $\mathcal{V}$ of $\mathcal{H}$ [11]. Since the inner product of $\mathcal{H}$ is not defined on $\mathcal{V}$, this leads to certain problems. Moreover, it is not *a priori* clear which enlargement to choose. For example, when $\hat{\varphi}_i$ is a second-order differential operator, a case which is of prime importance for quantum cosmology, there will be two linearly independent eigenfunctions Ψ_0^i, $i = 1, 2$, with eigenvalue zero. In cosmological models, where $\hat{\varphi}_i$ is the Wheeler-DeWitt operator (that is, the quantized super-Hamiltonian), the wave-function of the Universe is supposed to be a certain linear combination of Ψ_0^1 and Ψ_0^2. The formalism doesn't tell which combination to choose.

Partly in response to these problems, and partly on the basis of purely mathematical considerations, the author's method of constrained quantization singles out the second step of the classical symplectic reduction procedure as the one to be quantized. We will first review this method in its original formulation, and then introduce a refinement. Upon the latter, our method turns out to be surprisingly closely related to Dirac's method, applied to the enlargement $\mathcal{V}$, without sharing the difficulties just mentioned. A related approach is discussed by Marolf [12].

2 Quantized symplectic reduction

Applied to the special case of Marsden-Weinstein reduction of cotangent bundles, as above, our method amounts to choosing a dense subspace $\mathcal{E}$ of $L^2(Q)$

on which the quadratic form

$$(\Psi, \Phi)_0 = \int_G dx\, (\Psi, U(x)\Phi)_{L^2(Q)} \tag{1}$$

is well defined. Here U is a unitary representation of G on $L^2(Q)$ which quantizes the G-action on Q, and dx is a Haar measure on G. Unless G is compact, this form tends to be unbounded and even non-closable on $\mathcal{E}$, but one can nonetheless form the quotient $\mathcal{E}/\mathcal{N}$ of $\mathcal{E}$ by the null space $\mathcal{N}$ of $(\ ,\ )_0$. When the latter is positive semi-definite, $\mathcal{E}/\mathcal{N}$ is a pre-Hilbert space in the sesquilinear form inherited from $(\ ,\ )_0$. Its completion $\mathcal{H}^0$ is the physical state space of the constrained system, and as such serves as the quantization of classical reduced space $J^{-1}(0)/G = T^*(Q/G)$. This is true whether or not the Marsden-Weinstein quotient is regular.

The classical physical observables are functions F on T^*Q which Poisson-commute with the G-action. The quantization $\hat{F}$ of such an observable on the unphysical Hilbert space $L^2(Q)$ should commute with $U(G)$, and leave $\mathcal{E}$ stable. If these two conditions hold, $\hat{F}$ leaves $\mathcal{N}$ stable, and therefore quotients to an operator $\hat{F}^0$ on $\mathcal{E}/\mathcal{N}$. If $\hat{F}$ is bounded, $\hat{F}^0$ is bounded under suitable assumptions on G [8], and may be extended to $\mathcal{H}^0$ by continuity. When $\hat{F}$ is unbounded, containing $\mathcal{E}$ in its domain, this procedure yields an unbounded operator on the dense subspace $\mathcal{E}/\mathcal{N}$ of $\mathcal{H}^0$. The point is now that in typical examples $\hat{F}^0$ tends to be essentially self-adjoint on the projection $\mathcal{E}^0$ of $\mathcal{E}$ to $\mathcal{H}^0$. This is possible, because $\mathcal{E}^0$ is generally larger than $C_c^\infty(Q/G)$.

To see this in a simple example, classically due to Gotay and Bos [13], consider the standard action of $G = SO(2)$ on $Q = \mathbb{R}^2$. The momentum map for the pull-back action on $S = T^*\mathbb{R}^2$ is $J(p, q) = q \wedge p$, so that the quotient $J^{-1}(0)/SO(2)$ may be identified with $\mathbb{R}_0^+ \times \mathbb{R}$ (where $\mathbb{R}_0^+ := \mathbb{R}^+ \cup 0$), which may be thought of as the cotangent bundle $T^*\mathbb{R}_0^+$. Hence the singularity in the reduced space takes the form of a boundary.

Quantum reduction is done with $\mathcal{H} = L^2(\mathbb{R}^2)$ and $\mathcal{E} = C_c^\infty(\mathbb{R}^2)$. The unconstrained quantum Hamiltonian $\hat{H}_{\text{phys}} = -\Delta + V(r)$ on $L^2(\mathbb{R}^2)$ is $SO(2)$-invariant and essentially self-adjoint on $C_c^\infty(\mathbb{R}^2)$. Using the unitary transformation $U : L^2(\mathbb{R}^+, rdr) \to L^2(\mathbb{R}^+, dr)$ defined by $U\Psi(r) := \sqrt{r}\Psi(r)$, we have

$$U\hat{H}^0_{\text{phys}}U^* = -\frac{d^2}{dr^2} - \frac{1}{4r^2} + V(r). \tag{2}$$

While the analysis of this expression is quite straightforward for any reasonable potential V, the free case $V = 0$ already suffices to illustrate the main point.

Defined on $C_c^\infty(\mathbb{R}^+)$, the operator (2) is in the limit circle case [2] at 0 and in the limit point case [2] at ∞. Hence it has deficiency indices $(1, 1)$, so that it is

not essentially self-adjoint. However, defined on $\mathcal{E}^0 = C_c^\infty(\mathbb{R}^2)^0$, which consists of functions of the type $\Psi(r) = \sqrt{r} f(r^2)$ with $f \in C_c^\infty(\mathbb{R}_0^+)$, the operator in question is essentially self-adjoint, as follows from Thm. 3 in Nussbaum [14]. The closure of the latter operator is an extension of the closure of the former, to whose domain one adds functions of the indicated type in order to achieve essential self-adjointness. The boundary condition $\Psi(0) = 0$ corresponds to a hard wall potential at the origin.

Other examples of this phenomenon are given by Wren [15], who looks at the quantization of Stieffel chambers (i.e., quotients of a maximal torus of a compact Lie group by its Weyl group), finding that our procedure assigns Neumann boundary conditions to the Laplacian.

3 Minisuperspace quantum cosmology

Let us now apply our quantization method to the simplest cosmological models in minisuperspace. Using the canonical formalism (see our earlier work [9] for a covariant approach), we assume that the Hamiltonian constraint $H = 0$, in which H is a scalar, is the only constraint on the classical minisuper phase space. If the Hilbert space $\mathcal{H}$ results from the quantization of the unconstrained phase space, and the Wheeler-DeWitt operator $\hat{H}$ is the quantization of the Hamiltonian constraint (realized as an unbounded self-adjoint operator on $\mathcal{H}$), our formalism stipulates that firstly one should find a dense subspace $\mathcal{E} \subset \mathcal{H}$ on which the quadratic form

$$(\Psi, \Phi)_0 = \int_{\mathbb{R}} dt \, (\Psi, e^{itH} \Phi) \tag{3}$$

(cf. (1)) is well-defined. Secondly, one should determine the reduced Hilbert space $\mathcal{H}^0$, defined as in the preceding section. It would seem, therefore, that one needs to explicitly compute the null space $\mathcal{N}$ of $(\ ,\ )_0$. Fortunately, in practice there is often no need to do so. One may, instead, start from an *Ansatz* Hilbert space $\tilde{\mathcal{H}}^0$, and find a 'quantum reduction map' $V : \mathcal{E} \to \tilde{\mathcal{H}}^0$ satisfying

$$(V\Psi, V\Phi)_{\tilde{\mathcal{H}}^0} = (\Psi, \Phi)_0. \tag{4}$$

It is easily seen that V quotients and extends to a unitary isomorphism between $\mathcal{H}^0$ and $\tilde{\mathcal{H}}^0$, through which one may transfer the physical Hamiltonian and other observables from the unknown space $\mathcal{H}^0$ to $\tilde{\mathcal{H}}^0$, where everything is explicit [8]. The operators $\hat{A}$ on $\mathcal{H}$ that commute with $\hat{H}$ and leave $\mathcal{E}$ stable, are represented by physical observables $\hat{A}^0$ on $\tilde{\mathcal{H}}^0$ by the prescription

$$\hat{A}^0 V\Psi = V\hat{A}^0\Psi. \tag{5}$$

In the case at hand, these two steps may be taken at one stroke. Using the theory of eigenfunction expansions [3,16], one finds a Hilbert space $\mathcal{H}_-$ and a Hilbert-Schmidt injection $\mathcal{H} \hookrightarrow \mathcal{H}_-$, such that (almost) all *relevant* generalized eigenfunctions of $\hat{H}$ (that is, those contributing to the spectral resolution of $\mathcal{H}$) lie in $\mathcal{H}_-$. Hence $\mathcal{H}$ is a Hilbert subspace of $\mathcal{H}_-$ in the sense of Schwartz [17] (i.e., the embedding $\mathcal{H} \hookrightarrow \mathcal{H}_-$ is continuous). If $\mathcal{H}_+$ is the continuous dual of $\mathcal{H}_-$, one obtains an anti-linear map $\Psi \to \tilde{\Psi}$ from $\mathcal{H}_+$ to $\mathcal{H}$, defined by

$$\langle \Psi, \Phi \rangle = (\tilde{\Psi}, \Phi)_{\mathcal{H}} \tag{6}$$

for all $\Phi \in \mathcal{H}$. Here the restriction of $\Psi \in \mathcal{H}_+$ to $\mathcal{H} \subset \mathcal{H}_-$ (with its own Hilbert space topology) is continuous because of the continuity of the embedding $\mathcal{H} \hookrightarrow \mathcal{H}_-$; the Riesz-Fischer theorem then implies the existence of an element $\tilde{\Psi} \in \mathcal{H}$ for which (6) holds. The image $\tilde{\mathcal{H}}_+$ of $\mathcal{H}_+$ in $\mathcal{H}$ under this map is always dense, and when $\mathcal{H}$ is dense in $\mathcal{H}_-$, the map $\Psi \to \tilde{\Psi}$ is injective, so that $\mathcal{H}_+$ may be seen as a dense Hilbert subspace of $\mathcal{H}$. One then has a Gel'fand triplet (or rigged Hilbert space) $\mathcal{H}_+ \subset \mathcal{H} \subset \mathcal{H}_-$. However, it is by no means necessary that $\mathcal{H}$ be dense in $\mathcal{H}_-$, so that the formalism of Schwartz is a generalization of that of Gel'fand.

In case that the spectrum $\sigma(\hat{H})$ does not contain 0, the physical Hilbert space $\mathcal{H}^0$ determined by (6) is empty. When $\hat{H}$ has 0 in its discrete spectrum $\sigma_d(\hat{\mathcal{H}})$, so that the Wheeler-DeWitt equation $\hat{H}\Psi = 0$ has a solution $\Psi \in \mathcal{H}$, there is no need for our formalism. This rarely occurs in minisuperspace models; instead, we assume that 0 lies in the absolutely continuous spectrum $\sigma_{ac}(\hat{\mathcal{H}})$. We may take $\tilde{\mathcal{H}}^0$ as the corresponding multiplicity space, realized in some arbitrary fashion, with

$$V\tilde{\Psi}(\mu) = \overline{\langle \Psi, \varphi_\mu(0) \rangle}, \tag{7}$$

defined for $\Psi \in \mathcal{H}_+$, so that $\tilde{\Psi} \in \mathcal{E}$. Here $\varphi_\mu(\lambda)$, where $\lambda \in \sigma(E)$ and μ labels a basis of $\tilde{\mathcal{H}}^0$, is a generalized eigenfunction of $\hat{H}$ in $\mathcal{H}_-$ with generalized eigenvalue λ. Note that (7) is well defined, for the $\varphi_\mu(\lambda)$ lie in the closure of $\mathcal{H}$ in $\mathcal{H}_+$. One easily verifies (4) from (3) and eq. (1.17) in §V.1 of Berezanskii's book [3].

An operator $\hat{A}$ on $\mathcal{H}$ that leaves $\mathcal{H}_+$ stable has a dual $\hat{A}^* : \mathcal{H}_- \to \mathcal{H}_-$. If, in addition, $\hat{A}$ commutes with $\hat{H}$, the dual $\hat{A}^*$ cannot change the generalized eigenvalue λ, so that, in particular, one has $\hat{A}^*\varphi_\mu(0) = \hat{A}^*_{\mu\nu}\varphi_\nu(0)$ for certain coefficients $\hat{A}^*_{\mu\nu}$. Combining this with (7) and (5), we see that an observable $\hat{A}_{\text{phys}}$ on $\mathcal{H}$ is realized on the physical state space $\tilde{\mathcal{H}}^0$ by

$$\hat{A}^0_{\text{phys}} f(\mu) = \overline{\hat{A}^*_{\mu\nu}} f(\nu). \tag{8}$$

4 The wave-function of the Universe

Physical processes in the quantum Universe may be computed if one specifies the physical Hamiltonian; as pointed out before, this should be an operator $\hat{H}_{\rm phys}$ on the unconstrained Hilbert space $\mathcal{H}$ which commutes with the Wheeler-DeWitt operator $\hat{H}$, and leaves $\mathcal{H}_+$ stable. This operator induces an operator $\hat{H}^0_{\rm phys}$ on the physical Hilbert space $\tilde{\mathcal{H}}^0$, given by (8). One may anticipate that the spectrum of $\hat{H}^0_{\rm phys}$ is purely continuous, since otherwise the Universe would settle in its ground state, and nothing would happen.

For example, a classical homogeneous and isotropic universe filled with noninteracting dust may be described by the phase space $T^*\mathbb{R}^2$, with coordinates (α, ϕ) standing for the logarithm of the radius and the dust field, respectively, with conjugate momenta (p_α, p_ϕ). The classical super-Hamiltonian is

$$H_\kappa = \tfrac{1}{2}\left(p_\alpha^2 + \kappa e^{4\alpha} - p_\phi^2\right), \tag{9}$$

where $\kappa = 0$ or ± 1. A reasonable choice for the classical physical Hamiltonian is

$$H_{\rm phys} = p_\phi; \tag{10}$$

the idea is that the dust field serves as a physical time parameter [1], but since ϕ itself does not Poisson-commute with the constraint H_κ, this idea must be implemented through its conjugate p_ϕ, which does.

The unconstrained Hilbert space is simply $\mathcal{H} = L^2(\mathbb{R}^2)$, with wave-functions $\Psi(\alpha, \phi)$. The Wheeler-DeWitt equation

$$\tfrac{1}{2}\left(-(\partial/\partial\alpha)^2 + \kappa \exp(4\alpha) + (\partial/\partial\phi)^2\right)\Psi = 0 \tag{11}$$

can be solved explicitly for all values of κ [9]; we now add the knowledge that the *relevant* generalized eigenfunctions must be polynomially bounded [16] in order to contribute to the spectral resolution of $\mathcal{H}$. For $\kappa = 0$ this leads to $\tilde{\mathcal{H}}^0_0 = L^2(\mathbb{R}) \otimes \mathbb{C}^2$, whereas for $\kappa = \pm 1$ one has $\tilde{\mathcal{H}}^0_{\pm 1} = L^2(\mathbb{R})$. The generalized eigenfunctions at 0 are, omitting the argument (0),

$$\varphi^{\kappa=0}_{k,\pm}(\alpha, \phi) = \exp[ik(\alpha \pm \phi)]; \tag{12}$$

$$\varphi^{\kappa=1}_{k}(\alpha, \phi) = \pi^{-1} e^{i\phi k}\sqrt{\sinh(\pi|k|/2)}\,K_{i|k|/2}(\tfrac{1}{2}e^{2\alpha}); \tag{13}$$

$$\varphi^{\kappa=-1}_{k}(\alpha, \phi) = \tfrac{1}{2} e^{i\phi k}\sqrt{\operatorname{cosech}(\pi|k|/2)}\,(J_{i|k|/2} + J_{-i|k|/2})(\tfrac{1}{2}e^{2\alpha}). \tag{14}$$

With (10) as the physical Hamiltonian, it is reasonable to ask the wave-function of the Universe to peak around $k = 0$; this approximately yields $\Psi^{\kappa=0} \simeq 1$, $\Psi^{\kappa=1} \simeq K_0$, and $\Psi^{\kappa=0} \simeq J_0$. This agrees with Hartle-Hawking boundary conditions for $\kappa = -1$ only, and always disagrees with Vilenkin

boundary conditions (as imposed by Zhuk [18]). However, a direct comparison is difficult, because these authors use a mathematical framework unrelated to the theory of self-adjoint operators on a Hilbert space.

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